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ABSTRACT

This document is a monograph intended for advanced undergraduate students, or beginning graduate students, who have some knowledge of modern physics as well as classical physics, including the elementary quantum mechanical treatment of the hydrogen atom and angular momentum. The first chapter introduces symmetry and relates it to the mathematical concept of invariance under a transformation of variables. These ideas are illustrated in the context of the classical laws of mechanics in the Newtonian form. The emphasis here, as in the rest of the monograph, is directed toward physical, rather than mathematical, generality. The second chapter, which is only partly completed, and which will be revised in order to simplify the presentation, discusses symmetries of the Schrodinger equation for one or two particles, including gauge invariance of the wave function and parity. (Author/PR)

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The Symmetry of Natural Laws

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GENERAL PREFACE

This monograph was written for the Conference on the New Instructional Materials in Physics, held at the University of Washington in the summer of 1965. The general purpose of the conference was to create effective ways of presenting physics to college students who are not preparing to become professional physicists. Such an audience might include prospective secondary school physics teachers, prospective practitioners of other sciences, and those who wish to learn physics as one component of a liberal education.

At the Conference some 40 physicists and 12 filmmakers and designers worked for periods ranging from four to nine weeks. The central task, certainly the one in which most physicists participated, was the writing of monographs.

Although there was no consensus on a single approach, many writers felt that their presentations ought to put more than the customary emphasis on physical insight and synthesis. Moreover, the treatment was to be "multi-level" --- that is, each monograph would consist of several sections arranged in increasing order of sophistication. Such papers, it was hoped, could be readily introduced into existing courses or provide the basis for new kinds of courses.

Monographs were written in four content areas: Forces and Fields, Quantum Mechanics, Thermal and Statistical Physics, and the Structure and Properties of Matter. Topic selections and general outlines were only loosely coordinated within each area in order to leave authors free to invent new approaches. In point of fact, however, a number of monographs do relate to others in complementary ways, a result of their authors' close, informal interaction.

Because of stringent time limitations, few of the monographs have been completed, and none has been extensively rewritten. Indeed, most writers feel that they are barely more than clean first drafts. Yet, because of the highly experimental nature of the undertaking, it is essential that these manuscripts be made available for careful review

by other physicists and for trial use with students. Much effort, therefore, has gone into publishing them in a readable format intended to facilitate serious consideration.

So many people have contributed to the project that complete acknowledgement is not possible. The National Science Foundation supported the Conference. The staff of the Commission on College Physics, led by E. Leonard Jossem, and that of the University of Washington physics department, led by Ronald Geballe and Ernest M. Henley, carried the heavy burden of organization. Walter C. Michels, Lyman G. Parratt, and George M. Volkoff read and criticized manuscripts at a critical stage in the writing. Judith Bregman, Edward Gerjuoy, Ernest M. Henley, and Lawrence Wilets read manuscripts editorially. Martha Ellis and Margery Lang did the technical editing; Ann Widditsch supervised the initial typing and assembled the final drafts. James Grunbaum designed the format and, assisted in Seattle by Roselyn Pape, directed the art preparation. Richard A. Mould has helped in all phases of readying manuscripts for the printer. Finally, and crucially, Jay F. Wilson, of the D. Van Nostrand Company, served as Managing Editor. For the hard work and steadfast support of all these persons and many others, I am deeply grateful.

Edward D. Lambe
Chairman, Panel on the
New Instructional Materials
Commission on College Physics

THE SYMMETRY OF NATURAL LAWS

PREFACE

"The Symmetry of Natural Laws" is a monograph intended for advanced undergraduate students, or beginning graduate students, who have some knowledge of modern physics as well as classical physics, including the elementary quantum mechanical treatments of the hydrogen atom and angular momentum. Thus it could well form part of the instruction in the latter part of a course in introductory quantum theory.

The first chapter introduces the symmetry concept and relates it to the mathematical concept of invariance under a transformation of variables. These ideas are illustrated in the context of the classical laws of mechanics in the Newtonian form. The emphasis here, as in the rest of the monograph, is directed to physical, rather than mathematical, generality. The first chapter has been tested on some undergraduate students.

The second chapter, which is only partly completed, and will be revised in order to simplify the presentation, discusses the symmetries of the Schrodinger equation for one or two particles, including gauge invariance of the wave function and parity. The rest of the chapter will discuss statistics.

Chapters to be written will include charge independence, with application to nuclei and fundamental particles, and the unitary symmetries.

Laurie Brown

CONTENTS

1	THE SYMMETRY IDEA: APPLICATION IN CLASSICAL PHYSICS	1
1.1	Introduction	1
1.2	Positronium	2
1.3	Symmetry in nature	4
1.4	Consequences of the symmetry of natural laws	5
1.5	Symmetry and invariance	5
1.6	Reading a symmetry from a natural law	7
1.7	The "time-reversal" transformation	8
1.8	Inferring a law of nature from a symmetry	11
1.9	Symmetry, invariance, and conservation laws	11
2	SYMMETRY PRINCIPLES IN QUANTUM THEORY	13
2.1	Introduction	13
2.2	The free particle in quantum theory	14
2.3	Particle in a symmetric potential--parity	15
2.4	Two-particle systems in quantum mechanics	17
Appendix	GROUP ALGEBRA	20

1 THE SYMMETRY IDEA: APPLICATIONS IN CLASSICAL PHYSICS

1.1 INTRODUCTION

The concept of symmetry, as applied to the laws of physics, is an extension of geometrical symmetry which is illustrated, for example, by the equilateral triangle. We recognize the equilateral triangle ABC in Fig. 1.1(a) as possessing a symmetry not possessed by the scalene triangle A'B'C'. Let us try to express in words our feelings about the two triangles.

Given an exact duplicate of the equilateral triangle, we would not know which corner to label A. That is, the three corners are all equivalent. In more technical language, the triangle ABC can be brought into congruence with itself in three different ways through rotations in the plane by 120°. This is a threefold symmetry.

Having arbitrarily selected a corner to label A, there remain two ways of assigning the letters B and C. One way is shown in Fig. 1.1(a): A, B, C are assigned in order clockwise. However, they could have been assigned counterclockwise instead, and no rotation in the plane will convert the clockwise to the counterclockwise ordering. Notice that if we were viewing Fig. 1.1(a) from beneath the page, instead of from above, the ordering would have appeared counterclockwise. Therefore, flipping the triangle over will change the ordering (viewing it in a mirror will do the same). Having flipped it over, we can still rotate it through 120° and bring it into congruence, and then repeat this rotation to bring it into congruence still one more way. There are thus, if we permit flipping the triangle, six ways to bring it into congruence with itself, i.e., a sixfold symmetry. Only one of these six congruence operations, which are illustrated in Fig. 1.2, is possible for A'B'C', which has the lowest of all orders of symmetry, namely onefold (i.e., no symmetry).

Up to this point we have related

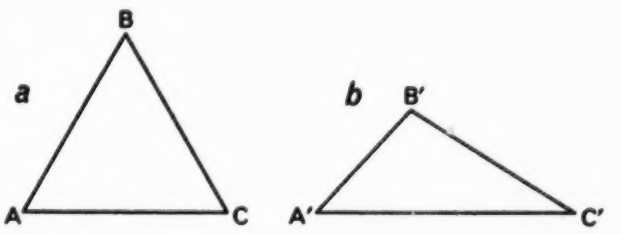


Fig. 1.1 Two kinds of triangles, (a) equilateral and (b) scalene.

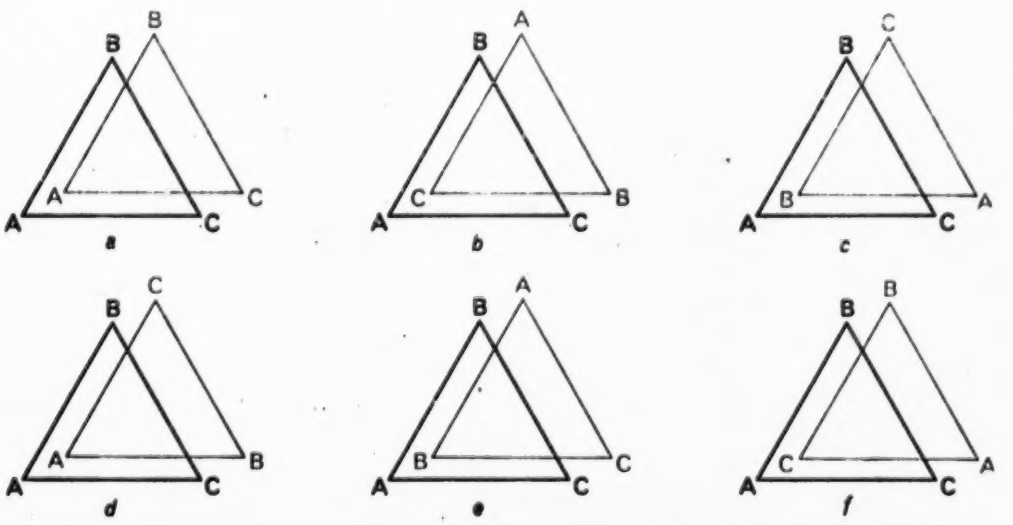


Fig. 1.2 Congruences of the equilateral triangle ABC.

the notion of symmetry to the set of congruences of two identical, labeled triangles and have used the ideas of rotation and flipping to make concrete the method for achieving such congruences. These operations are evidently not unique. For example, to achieve the congruence shown in Fig. 1.2(e) we could rotate the original triangle by some angle not 120°, then flip about any axis, then perform an appropriate rotation and sliding to bring it to the desired location. However, there is some point in selecting for study a set of simple operations, just sufficient to achieve all six congruences.

A minimum set of operations which bring the equilateral triangle into congruence with itself (and which we may call symmetry operations) such as rotations by 0°, 120°, 240°, etc., and "flipping" about some axis in the plane can be analytically described in a number of ways. The most powerful way of doing so is in terms of an abstract algebra of operations. For example, if I is the identity operation (that is, leaving the triangle alone - analogous to multiplying a number by the number 1) and if R is the operation of clockwise rotation by 120°, and if we write

$$R^3 = I, \qquad (1.1)$$

this means that three successive clockwise rotations of 120° are the same as leaving the triangle alone. The mathematical symbols R and I are called operators and an operator algebra like that satisfied by the congruence operations on the equilateral triangle is called a group algebra. We shall not explicitly use the group algebra concept in our work, but it is an interesting branch of mathematics which is briefly discussed in an elementary way in the Appendix.

A group of symmetry operations is analogously associated with any regular plane figure, such as the square, pentagon, hexagon, etc., and thus also for the circle, which is a limiting case of such regular n-sided figures. The circle exhibits a continuous sequence of congruences with itself (any point may be labeled A), and upon flipping a clockwise sequence of points becomes counterclockwise.

Regular solids, such as cubes and spheres, possess symmetry properties which can be discussed in a similar way, and such geometrical symmetries play an important role in much physical reasoning. The science of crystallography, for example, consists largely of the determination of this kind of symmetry and in its applications.

But the symmetry of physical laws is often less easily visualizable. To anticipate the sort of thing we are aiming at, consider the symmetry known as "charge independence of the nuclear forces." One example of this symmetry is furnished by the pi-mesons or pions. There are pions carrying electric charges of +e, 0, and −e, where −e is the charge of the electron. The charged and neutral pions have nearly the same mass and are regarded as different "charge states" of a single particle, the pion. As regards the role played by the pions in nuclear forces, the three charge states are essentially equivalent. Thus, in some sense, they resemble the three corners of the equilateral triangle. This necessarily vague description of "charge independence" will be made more precise after we become more familiar with symmetry concepts in physics.

To begin familiarizing ourselves, we start with a simple physical system consisting of a positive and a negative electron attracting each other by electrostatic forces.

1.2 POSITRONIUM

A positronium "atom" is a hydrogenlike system in which the proton is replaced by a positron. Unlike the proton, the positron has properties identical with the electron, except

We are assuming here that the structure of hydrogen-like atoms is entirely determined by the electrostatic Coulomb force. While this is an excellent first approximation, it is not entirely correct. Among the many smaller effects which we are neglecting are magnetic effects, relativistic effects, and those which are due to the internal structure of the negatively and positively charged particles. In positronium, an especially interesting effect is the "virtual annihilation" of the electron-positron pair forming a photon, which then materializes again into an electron-positron pair. Use of the words "then" and "again" as indicating a temporal sequence is in this case purely schematic, as in fact the details of this process are completely unobservable, though we know it must exist and must shift the energy levels. (Can you see why it cannot be observable? Can you estimate the size of some of the effects we have mentioned? Can you think of other hydrogenlike systems? Can you think of any other effects we have neglected?)

for the sign of its electric charge. (We note that because the charge of the positron is +e, its magnetic moment[1] $e\hbar/2m$ is positive, while that of the electron is $-e\hbar/2m$.)

Because the positron and electron are identical in mass, and since the designations "positive" and "negative" charge are purely conventional, the system is highly symmetrical in a way that hydrogen is not. However, we can see the relationship of the states of positronium to those of hydrogen, by starting with a hydrogen atom and imagining the proton to get lighter, until its mass is equal to that of the electron. Recall the expression for the energy of a hydrogen atom in the state of principal quantum number n (relative to an infinitely separated electron and proton):

$$E_n = -\frac{Ry(H)}{n^2}, \qquad (1.2)$$

where $Ry(H) = \mu e^4/2\hbar^2$ and the reduced mass μ is given by

$$\frac{1}{\mu} = \frac{1}{M} + \frac{1}{m}, \qquad (1.3)$$

M is the mass of the nucleus (in this case the proton), and m is the mass of the electron. [In the classical Bohr model, proton and electron revolve opposite each other about their common center of mass in such a way that their moment of inertia is $\mu\delta^2$, where δ is the distance between proton and electron. Can you prove this?]

From Eq. (1.2) it is clear that if M is very large compared to m, as in hydrogen, then μ is nearly equal to m. Also, the center of mass of the atom is very close to the proton. But if M is made smaller, the center of mass moves away from the positive charge until the positive and negative charge are symmetrically located with respect to it. Equation (1.3) becomes, when M = m,

$$\frac{1}{\mu} = \frac{1}{m} + \frac{1}{m} = \frac{2}{m}, \qquad (1.4)$$

so that $\mu = m/2$. The energy levels of positronium are thus identical with those given by Eq. (1.2), but with half half the spacing

$$E_n\ (\text{positronium}) = -\frac{Ry(\text{pos.})}{n^2} = -\frac{1}{2}\frac{Ry(H)}{n^2}. \qquad (1.5)$$

It is a remarkable fact that although electron and positron have identical properties, the matter of

[1] In mks units.

which our familiar universe is made contains only electrons. Of course, positrons feel a repulsive Coulomb force from positively charged protons and so would not form atoms, but particles identical to protons except for having a negative charge also exist, and have been produced by high energy beams from accelerators. They also constitute a rare component of the cosmic rays. These particles, called antiprotons, can form atoms with positrons which would be indistinguishable from ordinary hydrogen atoms except for the signs of their constituent charges. In fact, we know of no reason why an entire universe composed of antimatter might not exist.

Antiprotons and positrons (which can also be called antielectrons), in the presence of ordinary matter soon find their abundant oppositely charged counterparts and are attracted to them by the electrostatic Coulomb forces, antiprotons to protons or other atomic nuclei, and positrons to electrons. When this happens, each particle-antiparticle pair annihilates, the rest-mass-energy mc^2 being transformed in some other form of energy. Thus in our local universe, antimatter has a very short life.

1.3 SYMMETRY IN NATURE

The existence of particle-antiparticle pairs is a striking illustration of the fact that the underlying laws of nature, some of which are unknown to us, appear to possess important symmetry characteristics. Some of these symmetry properties can be read directly from known laws (for example, the laws of electrodynamics as we will see below), and we may, as a working hypothesis, guess that the unknown laws also possess these symmetries. Such a hypothesis must, of course, be subjected to experimental tests.

It is important to stress that we are talking about the symmetries possessed by the fundamental laws and the elementary constituents of matter (if, indeed, there be such), and that we cannot expect these symmetries to be apparent in ordinary uncontrolled observation. It is true that many symmetrical objects and processes appear in nature (such as nearly perfect single crystals), but they are exceptional. One reason for this is obvious. Consider two identical pendulums independently supported: if both are at rest, we have a completely symmetric system. But if one is set into motion, while the other remains at rest, the symmetry is destroyed. If, instead, the two pendulums are lightly coupled (say, with a weightless weak spring) and set into motion either exactly in phase or 180° out of phase with equal amplitudes, they will undergo symmetrical motions - but these initial conditions must be precisely chosen. Thus, symmetrical behavior of a system requires, in addition to the symmetry of the laws of nature, that the system be constituted and started in a symmetric way.

A lack of symmetry in "the way things got started" may be the reason why, although natural law (so far as we know) is symmetric between particle and antiparticle, ordinary matter is made entirely of particles - and not antiparticles. There is, however, another possibility. The symmetry laws which we read from a known law of physics, and which operate successfully on a given level of experience, may fail when subjected to a more sensitive test. Thus, for example, space-reflection symmetry (or "parity"), says that right-handed and left-handed descriptions of nature are equivalent. This holds for the electromagnetic and the strong nuclear interactions but has been found to fail for the weak interactions. It is, therefore, a useful approximate symmetry on a certain level of experience, but it is violated in some types of relatively rare processes. On the cosmological time scale, even a small violation of symmetry can have enormous effects. We do not know how much

of the lack of symmetry in nature is due to weak violations of the otherwise symmetrical laws of nature.

1.4 CONSEQUENCES OF THE SYMMETRY OF NATURAL LAWS

Among the many successes of theoretical physics after the development of quantum mechanics, perhaps the most spectacular have been the predictions of the existence of hitherto unknown fundamental particles and their properties. These predictions have been based to a large extent upon symmetry considerations. Dirac's wave equation, proposed in 1928 to give a relativistically correct description of the spinning electron, possesses symmetry under an operation (that is, a mathematical transformation), known as "charge conjugation", and this led to the prediction of the positron, discovered in the cosmic rays in 1934. Although Dirac's equation does not give a complete account of the electromagnetic properties of the proton, on the other hand, the assumption that the true laws governing the proton, whenever they are found, will also possess the property of charge conjugation symmetry similarly led to the prediction of the existence and other properties of the antiproton, discovered at Berkeley in 1955. Detailed discussion of Dirac's equation is beyond the scope of this monograph, and we shall confine ourselves to mathematically simpler examples. However, a discussion of charge conjugation invariance for particles without spin will be included in Appendix 2.

1.5 SYMMETRY AND INVARIANCE

Up to this point we have been using the term "symmetry" in a general intuitive sense. The mathematical meaning of symmetry is contained in the notion of invariance of a mathematical expression under a transformation of variables.

Suppose we have a mathematical expression depending on one or more variables u, v, w ,... and transform to a new set of variables equal in number u', v', w',... . That is, we have

$$u' = u'(u, v, w, \ldots)$$
$$v' = v'(u, v, w, \ldots). \qquad (1.6)$$

If the transformation is a suitable one, we will be able to solve these equations for the original variables and obtain

$$u = u(u', v', w', \ldots)$$
$$v = v(u', v', w', \ldots). \qquad (1.7)$$

[For example, we might have

$$u' = \frac{1}{\sqrt{2}}(u + v),$$
$$v' = \frac{1}{\sqrt{2}}(u - v), \qquad (1.8)$$

which can be solved to give

$$u = \frac{1}{\sqrt{2}}(u' + v')$$
$$v = \frac{1}{\sqrt{2}}(u' - v').] \qquad (1.9)$$

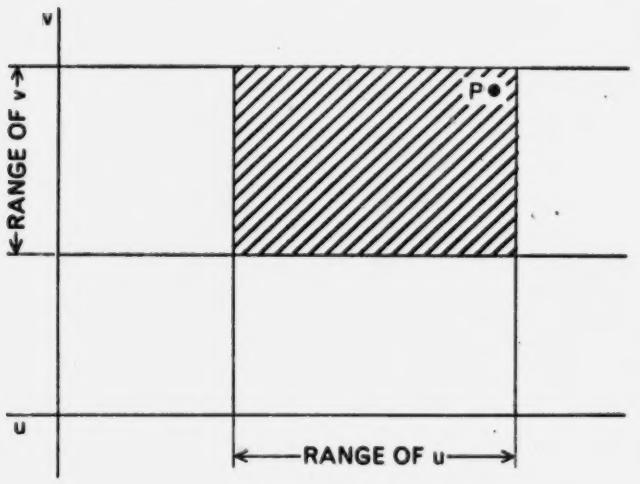
If we now transform our original methematical expression f(u, v, w,...) by substituting for u, v, w,... their expressions, Eq. (1.7), in terms of the new variables, we obtain a new and, in general, different function g of the new variables (which is, however, numerically equal to the old one):

$$f(u, v, w, \ldots) = g(u', v', w', \ldots). \qquad (1.10)$$

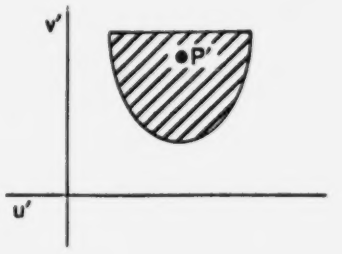
[For the example given in Eq. (1.8) and (1.9) we get

$$f(u, v) = f\left(\frac{1}{\sqrt{2}}(u' + v'), \frac{1}{\sqrt{2}}(u' - v')\right)$$
$$= g(u', v').] \qquad (1.11)$$

A convenient pictorial representation, very frequently used, is the following: Suppose there are only two variables u and v, each of which can take on a certain continuous range of numerical values. Let us set up a system of perpendicular u and v axes. A pair of allowed values of u and v corresponds to a point in the cross-



hatched area, and f(u, v) can be thought of as a number attached to this point. Similarly we can set up a set of u', v' axes and use Eq. (1.6) to determine a pair of values of u', v' for each pair u, v and in this way relate a point in the (u', v') plane to each allowed point in the (u, v) plane. In general, the area in the (u', v') plane will not resemble that in the (u, v) plane. The equality in Eq. (1.10) states that the number attached to the point P' in the (u', v') plane is the same as the number attached to its <u>corresponding</u> point P in



the (u, v) plane. This picture, which can be extended to more variables by introducing more dimensions, holds for any transformation of the kind we have called "acceptable.' (What sort of transformations might be "unacceptable?") Since the coordinates u', v' are usually different from the coordinates u, v, the function g(u', v') must usually be <u>different</u> from the function f(u, v) to attach the <u>same</u> number to the point P in the u, v plane and the point P' in the u', v' plane. If, nevertheless, as for the example discussed in Eqs. (1.8), (1.9), and (1.12), it turns out that while P' and P are given by different pairs of numbers, f(u, v) and g(u', v') give the same values <u>also</u> for the same pair of numbers, then f(u, v) is <u>invariant</u> under the transformation of u, v to u', v'. (Try a numerical example to illustrate these ideas.)

If now it should turn out that not only are f(u, v, w,...) and g(u', v', w',...) numerically equal, but that g is the <u>same</u> function of the primed variables that f is of the unprimed variables (obviously this is a very special circumstance), we then say that f(u, v, w,...) is <u>invariant</u> under the transformation of variables. Eq. (1.6).

[Again, for the example of Eq. (1.8), if

$$f(u, v) = u^2 + v^2, \qquad (1.12)$$

then

$$f\left(\frac{1}{\sqrt{2}}(u' + v'), \frac{1}{\sqrt{2}}(u' - v')\right)$$

$$= \frac{1}{2}(u' + v')^2 + \frac{1}{2}(u' - v')^2$$

$$= u'^2 + v'^2 = g(u', v'). \qquad (1.13)$$

Thus, not only does

$$f(u, v) = g(u', v'), \qquad (1.14)$$

which merely expresses the numerical equality of the expressions f and g

for corresponding values of the variables u, v of f and the variables u', v' of g (i.e., those values related by Eq. (1.5) or their equivalent Eq. (1.16); but also

$$g(u', v') = f(u', v'). \qquad (1.15)$$

This makes the much stronger statement that g has the same form in the variables u', v', that f has in the variables u, v. That is, g and f are the same functions of their respective variables.

A type of transformation which plays a very important role in many physical applications is the linear transformation of a set of variables, say, $u_1 \ldots u_n$ to a set of variables $u_1' \ldots u_n'$:

$$\begin{aligned} u_1' &= a_{11}u_1 + a_{12}u_2 + \ldots + a_{1n}u_n \\ u_2' &= a_{21}u_1 + a_{22}u_2 + \ldots + a_{2n}u_n \\ &\ldots\ldots \\ u_n' &= a_{n1}u_1 + a_{n2}u_2 + \ldots + a_{nn}u_n \end{aligned} \qquad (1.16)$$

The set of numerical coefficients $\{a_{ij}\}$ is often written as a square array

$$\begin{vmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{21} & a_{22} & \ldots & a_{2n} \\ & \ldots\ldots & & \\ a_{n1} & a_{n2} & \ldots & a_{nn} \end{vmatrix} \qquad (1.17)$$

and is called a matrix.

1.6 READING A SYMMETRY FROM A NATURAL LAW.

As a simple example from classical physics, let us take Newton's second law, restricting it to one space dimension,

$$F = ma = m\ddot{x}. \qquad (1.18)$$

By x is meant the position, with respect to some origin, of a classical Newtonian point particle of mass m, while $\ddot{x}$ stands for d^2x/dt^2. In general, then, x will be a function of the time $x = x(t)$. The force F applied to the particle can be arbitrarily chosen in this model, and whether or not Eq. (1.18) incorporates a symmetry depends entirely on the way the force depends on space and time or on the position of the particle.[2] We write Eq. (1.13) in the form

$$f(x, t) \equiv F(x, t) - m\ddot{x}(t) = 0, \qquad (1.19)$$

and consider the transformations of the variables x and t which leave f(x, t) invariant, for special choices of F.

Case (a). The force depends on t, but not on x.

In this case, the transformation

$$\begin{aligned} x' &= x - c, \\ t' &= t, \end{aligned} \qquad (1.20)$$

leaves f(x, t) invariant. For, solving for x and t, we get

$$\begin{aligned} x &= x' + c \\ t &= t', \end{aligned} \qquad (1.21)$$

and substituting in

$$f(x, t) = F(t) - m\frac{d^2x}{dt^2}, \qquad (1.22)$$

we get

$$\begin{aligned} g(x', t') &= f(x' + c, t') \\ &= F(t') - m\frac{d^2x'}{dt'^2} \\ &= f(x', t'). \end{aligned} \qquad (1.23)$$

The expression (1.22) for f(x, t) is

---

[2] Note that x (and also t) are being used with two different meanings which should, however, cause no confusion since the context will make clear which meaning is intended. We use x to designate a point in space and also to designate the position of a particle. In the former use dx/dt has no meaning (unless the whole coordinate system is moving); in the latter use, dx/dt is the velocity of the particle with respect to the fixed coordinate system.

thus invariant under the transformation Eq. (1.20). We have <u>also</u>, from Eq. (1.19)

$$g(x', t') = 0, \tag{1.24}$$

but this would be true even for transformations which do <u>not</u> leave Eq. (1.19) invariant, as this is already implied in the definition of "transformation." For example, consider the transformation

$$x' = x/b, \text{ or } x = bx',$$
$$t = t'. \tag{1.25}$$

Then,

$$g(x', t') = f(bx', t')$$
$$= F(t') - mb\ddot{x}'. \tag{1.26}$$

This is not equal to $f(x', t')$, unless $b = 1$. Nevertheless, $g(x', t') = 0$.

We may ask now, what is the meaning of the transformation Eq. (1.20)? This may be seen in Fig. 1.3.

Here x is the position of the particle with respect to the origin O, while $x' = x - a$ is the position of the particle with respect to the point a. Thus Eq. (1.22) is invariant with respect to a shift of the origin. This is, for this physical problem we can choose our origin anywhere. The motion of the particle is the same, no matter <u>where</u> we start it out. This will not be true in the next case considered.

Case (b). <u>The force depends on x, but not on t</u>.

In this case we write

$$f(x, t) = F(x) - m\ddot{x} \tag{1.27}$$

and consider the transformation

Fig. 1.3 Depiction of Eq. (1.20).

$$x' = x$$
$$t' = t - t_0. \tag{1.28}$$

We now obtain

$$g(x', t') = f(x', t' + t_0)$$
$$= F(x') - m\ddot{x}', \tag{1.29}$$

so that Eq. (1.27) is invariant to a shift of the origin of time; i.e., it does not matter when we start our stop watch. The motion of the particle is the same no matter <u>when</u> we start it.

An exceedingly simple, but very interesting transformation of Eq. (1.27) is

$$x' = x$$
$$t' = -t, \tag{1.30}$$

which is called "time-reversal." This gives

$$g(x', t') = F(x')$$
$$- m \frac{d}{d(-t')}\left(\frac{d}{d(-t')}\right)x' \tag{1.31}$$
$$= F(x') - m\ddot{x}' = f(x', t'),$$

so that again Eq. (1.27) is invariant. The physical meaning of the time-reversal transformation is by no means obvious, but its implications are profound and will be discussed in the next section.

1.7 THE "TIME-REVERSAL" TRANSFORMATION

When we discuss the symmetry of natural laws, we have in mind a region of space and an interval of time within which natural objects interact by means of their mutual forces. Whether we are considering a problem of relativistic dynamics, or one in which the nonrelativistic approximation is nearly correct, it is useful to adopt the idea of a maximum signal velocity so that we can observe our system within a region of space and an inter-

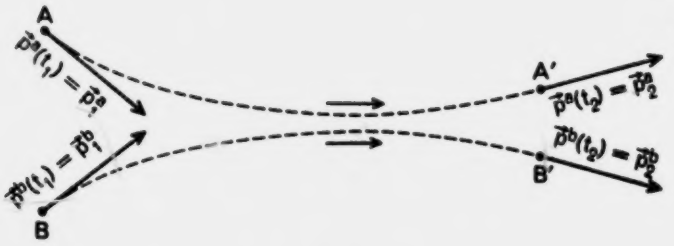


Fig. 1.4 Scattering of two particles.

Fig. 1.5 Impulse equals change of momentum.

val of time (or, as we say, a region of space-time), such that the system can be considered isolated. The important point is that we wish to avoid, at least for the time being, having to make assumptions about external forces.

Our isolated system is then a small universe. There are no forces "external" to this universe, and we may observe in it the free play of natural laws.

Consider now the collision of two particles in an isolated region of space-time, assuming the velocities are small enough that the nonrelativistic approximation holds. At the initial time t_1, let particle a have momentum $\vec{p}_1^{\,a}$ and let particle b have momentum $\vec{p}_1^{\,b}$, recalling that momentum $\vec{p} = mv = m(d/dt)\vec{r}$. These two momenta, $\vec{p}_1^{\,a}$ and $\vec{p}_1^{\,b}$, determine a plane which will be the plane of the subsequent motion, assuming that the mutual interaction forces act along the line joining the two particles, as is required by Newton's third law. In the course of time the mutual interaction forces $\vec{f}^{\,a}$ and $\vec{f}^{\,b}$, where $\vec{f}^{\,a} = -\vec{f}^{\,b}$, alter the momentum of each particle according to Newton's second law, i.e.,

$$\vec{f}^{\,a}(t) = \frac{d}{dt}\,\vec{p}^{\,a}(t) \qquad (1.32a)$$

$$\vec{f}^{\,b}(t) = \frac{d}{dt}\,\vec{p}^{\,b}(t), \qquad (1.32b)$$

so that by time t_2, the respective momenta have become $\vec{p}_2^{\,a}$ and $\vec{p}_2^{\,b}$ as shown in Fig. 1.4.

Since $\vec{p}^{\,a}$ and $\vec{p}^{\,b}$ are themselves time derivatives of the space coordinates of the particles, the transformation $t' = -t$ results, at any time t, in

$$\vec{p}^{\,a}(t') = \vec{p}^{\,a}(-t) = -\vec{p}^{\,a}(t) \qquad (1.33a)$$

and

$$\vec{p}^{\,b}(t') = \vec{p}^{\,b}(-t) = -\vec{p}^{\,b}(t). \qquad (1.33b)$$

> Under the time-reversal transformation the vector momentum and velocity of a particle change sign.[3]

The tangents to the particle trajectories in Fig. (1.4) give the directions of the momenta of particles a and b at each instant of time during their motion. The effect of the forces is to bring about a continuous change in these momenta. In a short time interval Δt, for example, Eq. (1.32) states that the changes in the momenta are

$$\Delta\vec{p}^{\,a}(t) = \vec{f}^{\,a}(t)\Delta t \qquad (1.34a)$$

$$\Delta\vec{p}^{\,b}(t) = \vec{f}^{\,b}(t)\Delta t. \qquad (1.34b)$$

This is the statement that <u>impulse equals change of momentum</u>. Notice that although we have labeled the forces by the time $\vec{f}^{\,a}(t)$, the forces in fact depend only on the <u>distance</u> between the particles. The meaning of Eq. (1.34a) can be exhibited graphically as in Fig. 1.5. Under the trans-

[3] Recalling that at each instant of time $\vec{f}^{\,a}(t) = -\vec{f}^{\,b}(t)$, we can infer from Eq. (1.32) that $(d/dt)\vec{p}_a(t) = -(d/dt')\vec{p}_b(t')$, where t' is <u>any transformation</u> of t, $t' = t'(t)$. This statement has obviously nothing to do with time-reversal-invariance even if we choose $t' = t'(t) = -t$.

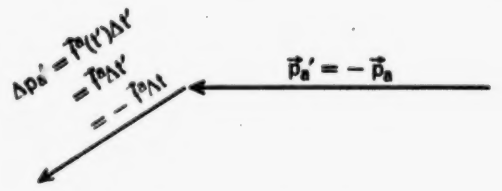


Fig. 1.6 Impulse equals change of momentum (time reversed).

formation $t' = -t$, the situation is graphically shown in Fig. 1.6. Thus, while $\vec{p}^a$ acquires the change of momentum $\Delta\vec{p}^a$, the fact that the laws of motion, Eq. (1.34), are invariant under the time-reversal transformation means that with the time reversed, $\vec{p}^{a\prime} = -\vec{p}^a$ acquires the change of momentum in an equal time interval of $\Delta\vec{p}^{a\prime} = -\Delta\vec{p}^a$. Note that it is essential here that the <u>force</u> is unchanged by the transformation.

Clearly, this means that if t_2 is <u>earlier</u> than t_1, and if we start at A' and B' instead of A and B (see Fig. 1.4), with momenta $-\vec{p}_2^{\,a}$ and $-\vec{p}_2^{\,b}$, the trajectories will be traversed in the reverse directions, the particles ending at A and B after a time equal to that for the forward traversal with momenta $-\vec{p}_1^{\,a}$ and $-\vec{p}_1^{\,b}$. In brief, <u>the motions are reversed</u>.[4]

Let us summarize what we have learned of the significance of the time-reversal transformation in classical mechanics:

When two particles obeying Newton's laws move under the action of their mutual interaction forces, if at any instant the momenta of the two particles are reversed, the reverse motion will result.

Thus, in a gas, where we consider a collection (or "ensemble") of random motions, we always ascribe an equal probability to a motion and its reversed motion. This is known as the <u>principle of detailed balance</u>.

More complex, though equally important, situations arise in classical physics than the collision of two Newtonian particles interacting by means of velocity independent forces depending only on the distance between particles. Nevertheless, it is found that the fundamental laws are always time-reversal invariant. This can always be interpreted, as we have done, as <u>motion reversal</u>: The final configuration with reversed momenta leads, with unchanged laws of force, to the initial configuration with reversed momenta, after an equal time interval. ("Initial" and "final" can, of course, designate any earlier and later time during the motion.)

In classical physics this leads to a certain paradox concerning the approach to equilibrium, which is not fully resolved even in the quantum theory. If we introduce some gas into one corner of a large evacuated box, we expect the gas to distribute itself uniformly throughout the volume. After a time T, it will then find itself in a certain configuration with the gas particles having definite momenta (in classical physics). At equilibrium, the configuration with reversed momenta is equally probable. But if this configuration is realized, it will lead after another interval T, to all the gas being again in the corner into which it was originally introduced. In the real gas, this does not happen, for small uncontrolled external influences cannot be entirely eliminated (vibrations of the support, sound waves, etc.). Since these belong to a larger universe than the box of gas, we become involved with a larger time scale than that of the gas molecule collisions. If, indeed, time-reversal invariance really holds exactly[5] and

[4] The transformation $t' = -t$ is a purely mathematical one, and there is no way, of course, to carry out this operation physically. It tells us something about the symmetry of the <u>equations</u> of physics. The physical analogy to keep in mind is this: If we take a movie of a process and run it backwards and the process is time reversal invariant, there is no way to tell with certainty whether we are seeing the original or the reversed motion, since both are possible motions.

[5] Recent experiments on the decay properties of K mesons appear to indicate the first evidence for possible <u>failure</u> of time-reversal invariance on a microscopic scale.

our universe is expanding into a "box", it may sometime reverse itself.

1.8 INFERRING A LAW OF NATURE FROM A SYMMETRY

Galileo's law of inertia, which is Newton's first law of motion, is fundamental to classical mechanics. This law states that in the absence of a net external force, the total momentum of a system is unchanged. At first sight, this may appear to be merely a special case of Newton's second law, but in fact the second law has no meaning unless the law of inertia holds, because otherwise Newton's second law becomes only a definition of what is meant by force, and thus has no predictive value. The law of inertia describes the setting within which the action takes place - namely, empty space. It permits the measurement of forces by balancing an unknown force against a standard force, since it gives a method for determining when no net force acts.

Consider a large, flat, horizontal, frictionless table top. Let us start an object from the center with a certain momentum. Until the edge is reached, no net forces will act to change the momentum. But if the table is curved, tipped, or rough, or contains holes, the momentum will not be conserved. Similarly, a three-dimensional space in which Newton's first law holds contains no roughness, curvature, edges, or other local features to disturb the motion. In brief, the space in which the law of inertia holds is homogeneous and isotropic; that is, each part of empty space is like each other part, and every direction is equivalent to every other direction. This is a symmetry. We have made the tacit assumption, as well, that each interval of time ("empty" time, if you like), has the same intrinsic properties as every other equal interval of time.

Can we reverse the discussion, and infer the law of inertia from the homogeneity of space and time, and the isotropy of space? Let us use the idea of invariance, considering a one-dimensional example. At some instant, let the position of a point particle be x and its velocity v. Assuming $v = v(x)$ and making the substitution $x' = x - x_0$, corresponding to a shift of origin, we get (refer to Eq. (1.14) and Eq. (1.15)),

$$v(x) = v(x' + x_0) \equiv v'(x'). \quad (1.35)$$

Because of the assumed homogeneity of space, the function v(x) must be invariant under the translation of the origin, hence

$$v'(x') = v(x') \quad (1.36)$$

and from Eq. (1.35) and Eq. (1.36) together, we have

$$v(x' + x_0) = v(x') \quad (1.37)$$

for <u>any</u> x_0. Hence the function v(x) must be a constant, which proves the law of inertia for this case. Because of the isotropy of space, this holds for any velocity component, and for $\vec{v} = \vec{v}(x, y, z)$.

1.9 SYMMETRY, INVARIANCE, AND CONSERVATION LAWS

In the previous section we have illustrated, for a very simple example, how a symmetry (the homogeneity and isotropy of space) can lead to invariance of an observable quantity (the invariance of the velocity v(x) considered as a function of the position x under an arbitrary shift of origin), and to the conclusion that p must be constant for the motion considered.

The statement that some measurable physical quantity does not change during a process undergone by some isolated system is a <u>conservation statement</u>. Of greatest interest are those quantities which can be identified as <u>never</u> changing for an isolated

system, whatever the process. Some examples are: total vector momentum, total angular momentum, total energy, total electric charge. These conservation laws can usually be shown to follow from a symmetry assumption. Aside from its great practical importance, this is a very interesting and esthetically satisfying realization.

QUESTIONS

1. Would you expect magnetic effects to be more or less important within the positronium atom than in the hydrogen atom? Why?

2. The mean time for the ground state of positronium to annihilate into two γ rays is about 10^{-10} sec. Is this a long or a short time on the atomic scale? Discuss.

3. Extend the discussion of the invariance properties of Eq. (1.19) by considering a general force F(x, t), depending on <u>both</u> space and time. If invariance is to be maintained under the transformation Eq. (1.21), what property must F possess? Under transformation Eq. (1.25)? Under transformation Eq. (1.28)? Under transformation Eq. (1.30)?

4. Can we show, using the arguments of section 1.8, that in a homogeneous, isotropic, force-free space the acceleration is constant as well as the velocity? What constant value has the acceleration?

2 SYMMETRY PRINCIPLES IN QUANTUM THEORY

2.1 INTRODUCTION

Symmetry principles play a much greater role in quantum physics than they do in classical physics. Among the many reasons are these:

(a) The classical laws are known. Thus, while the recognition of the symmetries they contain is esthetically satisfying, and often provides a powerful analytic tool, the laws in themselves are already complete and nothing essentially new is added. In those parts of quantum theory where the laws are either unknown or uncertainly known, one often tries to find those predictions which follow only from accepted symmetry principles and conservation laws.

(b) Classical physics can be considered as a special application of quantum physics when the constant of action h, Planck's constant, is negligible. In the limiting case, when $h \to 0$, the separation between states of definite energy tends to zero, so that a classical state is essentially an ensemble of many quantum mechanical states. For example, a magnet in a uniform magnetic field takes up one of only a finite set of discrete orientations in quantum theory, while in the classical limit the set of possible orientations is continuous. These two kinds of symmetry (discrete vs. continuous) are different. When the number of possible orientations is small, as in the quantum theory of elementary systems, powerful restrictions can be placed on the possible internal complexity of the system, while in classical theory this is not possible.

(c) The systems studied by quantum theory are usually simpler systems - such as crystals, molecules, atoms, nuclei, and elementary particles. The intrinsic symmetries of such systems are more readily apparent.

(d) There are many more quantum mechanical symmetries.

Reasons (b), (c), and (d) are not all independent of each other, and will require fuller explanation, particularly (d), which we now discuss.

Although the aim of quantum theory is to predict the results of experiment, there are intermediary stages of calculation when we deal with descriptions of the system which are not directly measurable. The features of the description which are not directly measurable have only a conventional significance like the labels A, B, C on the vertices of an equilateral triangle - and this gives rise, as in the case of the triangle, to a group of symmetry transformations.

Consider the Schrödinger wave function $\psi(\vec{r}, t)$, describing a particle in a potential. The physical significance of ψ is that its absolute square represents the probability (or sometimes only the relative probability) of finding the particle within a given volume. More precisely,

$$P(\vec{r}, t)dV \equiv |\psi(\vec{r}, t)|^2 dV \equiv \psi^*(\vec{r}, t)\psi(\vec{r}, t)dV \quad (2.1)$$

is the probability for finding the particle in the infinitesimal volume dV at the time t. But exactly the same information is contained in

$$\psi'(\vec{r}, t) = e^{i\varphi}\psi(\vec{r}, t), \quad (2.2)$$

since

$$|\psi'(\vec{r}, t)|^2 = |\psi(\vec{r}, t)|^2 \quad (2.3)$$

as long as φ is a real number. In fact, φ may be any arbitrary real function of space and time. This group of symmetry transformations of the wave function is called gauge transformation. The only other restriction on φ

The term "gauge invariance" is also used in connection with the classical electromagnetic field. In that case it is connected with the fact that, just as the static electric field $\vec{E}$ can be derived from a scalar potential V, $\vec{E} = -\text{grad } V$, so the static magnetic field $\vec{B}$ can be derived from a vector potential $\vec{A}$, according to

$$\vec{B} = \text{curl } \vec{A}.$$

However, since for any scalar function $\chi(\vec{r}, t)$, curl div $\chi \equiv 0$,

$$\vec{A}' = \vec{A} + \text{grad } \chi$$

is a vector potential which furnishes the same magnetic field as $\vec{A}$:

$$\vec{B} = \text{curl } \vec{A} = \text{curl } \vec{A}'.$$

This is referred to as "gauge invariance of the first kind," while that of the wave functions is called "guage invariance of the second kind." By using both gauge invariances and making the function χ identical with the function ϕ in Eq. (2.2) one can prove the conservation of electric charge in quantum theory.

is that if we add two wave functions, such as $\psi_1(\vec{r}, t) + \psi_2(\vec{r}, t)$, to form a new state, under a gauge transformation both $\psi_1(\vec{r}, t)$ and $\psi_2(\vec{r}, t)$ must undergo a gauge transformation with the same gauge function φ - otherwise the probability meaning will be altered.

To see this, consider a special example of the gauge transformation, obtained by letting φ be the number π. Since $e^{i\pi} = -1$, the transformation is

$$\psi'(\vec{r}, t) = -\psi(\vec{r}, t). \qquad (2.4)$$

Evidently $-\psi_1 - \psi_2$ has the same probability meaning as $\psi_1 + \psi_2$, while $-\psi_1 + \psi_2$ does not, for example.

The probability density $P(\vec{r}, t)$ is invariant under a gauge transformation of the wave function.

2.2 THE FREE PARTICLE IN QUANTUM THEORY

The simplest example of the Schrödinger wave equation is that for a free particle of energy E in one dimension:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x). \qquad (2.5)$$

A solution of this equation is

$$\psi(x) = C \exp \frac{ipx}{\hbar}, \qquad (2.6)$$

where C is a normalization constant and $p = \sqrt{2mE/\hbar^2}$. The relative probability of finding the particle between x and $x + \Delta x$ is

$$\int_x^{x+\Delta x} |\psi(x')|^2 dx' = |C|^2 \int_x^{x+\Delta x} dx' =$$

$$= |C|^2 \, \Delta x, \qquad (2.7)$$

i.e., proportional to the size of the interval Δx.

If we shift the origin of x to x_0 so that the new x value is $x' = x - x_0$, the wave function becomes

$$\psi(x) = \psi'(x') = C \exp \frac{ip(x' + x_0)}{\hbar}$$

$$= \exp \frac{+ipx_0}{\hbar} \psi(x') \qquad (2.8)$$

Thus the wave function is not invariant under a shift of origin. However, by applying the gauge transformation $\exp \frac{ipx_0}{x}$ to $\psi'(x)$ we get

$$\exp \frac{-ipx_0}{\hbar} \psi(x)$$

$$= \exp \frac{-ipx_0}{\hbar} \exp \frac{+ipx_0}{\hbar} \psi(x')$$

$$= \psi(x') \qquad (2.9)$$

so that the probability density P(x)

is not altered by the shift of origin. This corresponds to the fact that the motion of a free particle in classical mechanics is independent of the origin of coordinates. In each case, the result depends on the fact that the momentum is constant, since if p depended upon x the conclusion would not be valid.

2.3 PARTICLE IN A SYMMETRIC POTENTIAL PARITY

The Schrödinger equation for a particle of energy E bound in a potential is, in one dimension,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x).$$

In terms of the constant nonrelativistic total energy E and the potential energy V(x), the statement that the particle is bound in the potential means that the kinetic energy $T(x) = E - V(x)$ is negative for infinite separation, i.e., $T(x = \infty)$ and $T(x = -\infty)$ are negative. Many, though not all, potentials go to zero at infinity; for example, the Coulomb, gravitational, and square well potentials. For these cases "bound" is equivalent to E being negative.

Not all potentials need be symmetric about the origin. An energy diagram for a particle bound in a nonsymmetric potential is shown in Fig. 2.1.

If, however, the potential is symmetric about the origin (or better, if an origin can be found about which the potential is symmetric), as in Fig. 2.2, then interesting results follow about the nature of the wave function $\psi(x)$ which depend only on the symmetry and not on other details of the potential.

The symmetry of the potential about the origin means

$$V(x) = V(-x). \qquad (2.10)$$

If, then, we make the transformation of the variable x which corresponds to reflection about the origin

$$x' = -x, \qquad (2.11)$$

and substitute it in the Schrödinger equation, we get

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(-x)}{dx^2} + V(x)\psi(-x) = E\psi(-x). \qquad (2.12)$$

For one-dimensional problems in quantum mechanics it is easy to prove that there can be only one bound state of a given energy, and since $\psi(x)$ and $\psi(-x)$ both satisfy the same Schrödinger equation for a bound state of energy E, we know they must both describe the same physical situation. As discussed in the previous section,

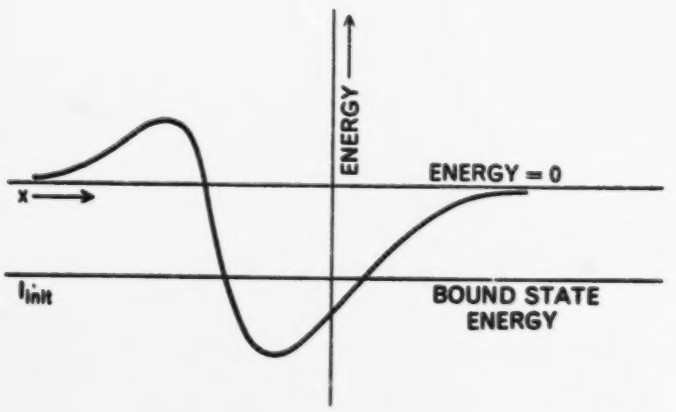


Fig. 2.1 Nonsymmetric potential.

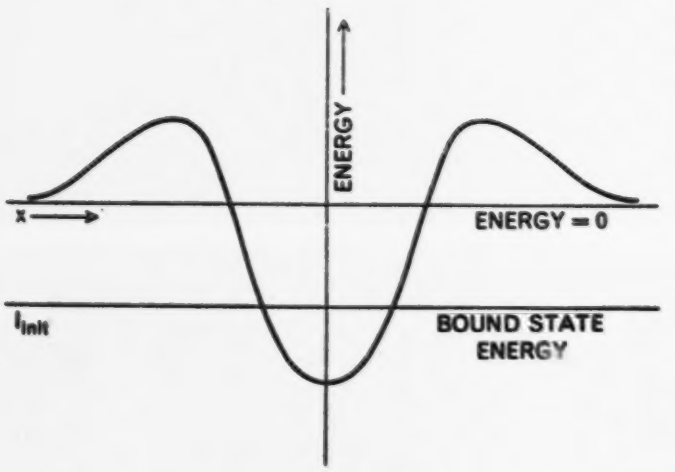


Fig. 2.2 Symmetric potential.

this means that the respective probability densities

$$P(x) = |\psi(x)|^2 \qquad (2.13)$$

and

$$P(-x) = |\psi(-x)|^2 \qquad (2.14)$$

must be equal. This, in turn, means

$$\psi(-x) = e^{i\phi}\psi(x) \qquad (2.15)$$

for all x. Thus,

$$\psi(-3) = e^{i\phi}\psi(3) \qquad (2.16)$$

but also

$$\psi(3) = e^{i\phi}\psi(3). \qquad (2.17)$$

That is, we can equally well write

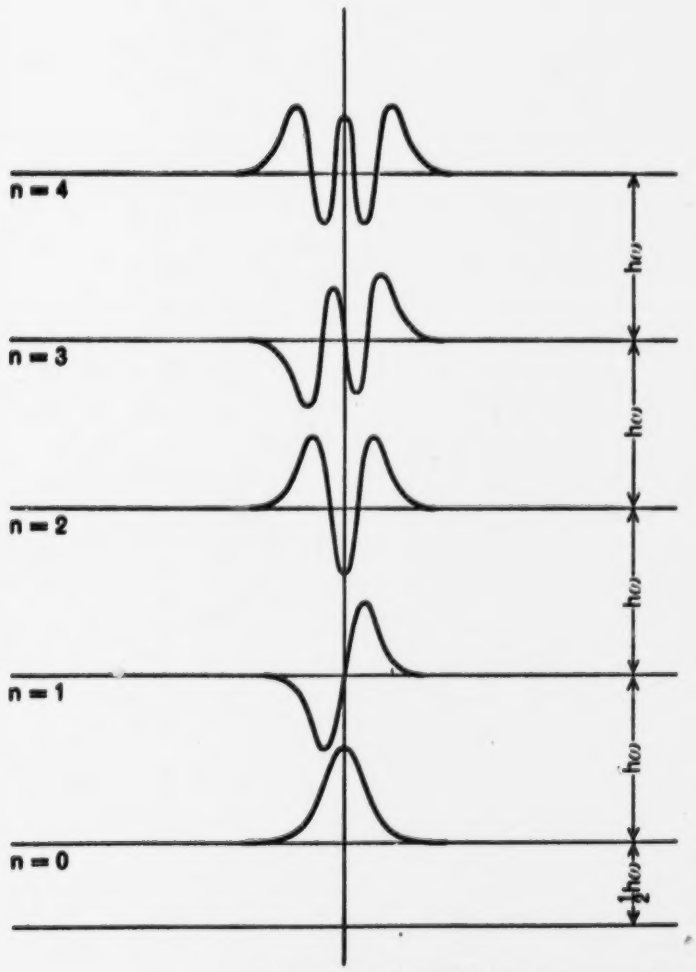


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Fig. 2.3 Wave functions for the one-dimensional harmonic oscillator.

(and this is <u>not</u> transformation of variables),

$$\psi(x) = e^{i\phi}\psi(-x). \qquad (2.18)$$

Substituting Eq. (2.15) in Eq. (2.18), we get

$$\psi(x) = e^{2i\phi}\psi(x) \qquad (2.19)$$

for all x, and hence

$$e^{2i\phi} = 1. \qquad (2.20)$$

Since $e^{2i\phi}$ is the square of $e^{i\phi}$, it follows that $e^{i\phi}$ is either +1 or −1, and we conclude from Eq. (2.15) or Eq. (2.18) that

$$\psi(x) = \pm\psi(-x). \qquad (2.21)$$

Now $\psi(x) = \psi(-x)$ means that the <u>wave function</u> has the same symmetry as the potential; that is, it is symmetric about the origin. The other solution,

$$\psi(x) = -\psi(-x), \qquad (2.22)$$

means that the wave function is antisymmetric about the origin (that is, the reflection is flipped over). Putting x = 0 in Eq. (2.22) we see that in the antisymmetric case the wave function must be <u>zero</u> at the origin.

Wave functions for the lowest energy levels of the symmetric harmonic oscillator potential $V(x) = \frac{1}{2}m\omega^2x^2$ are shown in Fig. 2.3. Notice that the ground state ($E = \frac{1}{2}\hbar\omega$) must be symmetric, as it has no nodes, and that the symmetric and antisymmetric (or <u>even</u> and <u>odd</u>), wave functions alternate as the energy is increased.

In three dimensions, reflection in the origin takes the form

$$\begin{aligned} x &\to -x \\ x &\to -y \\ z &\to -z \end{aligned} \qquad (2.23)$$

in Cartesian coordinates, or in vector terminology

$$\vec{r} \to -\vec{r}. \qquad (2.24)$$

This is known as the parity transformation. A function which is invariant under this symmetry transformation is said to have even parity, or parity +1. A function which becomes its own negative is said to have odd parity, or parity −1.

For example,

$$\cos\theta = \frac{z}{|\mathbf{r}|}, \quad |\mathbf{r}| = \sqrt{x^2 + y^2 + x^2} \tag{2.25}$$

has odd parity (although it is an even function of θ), while

$$\sin\theta = \sqrt{1 - \cos^2\theta} \tag{2.26}$$

has even parity. Similarly, a wave function in three dimensions which depends only on the length of $\vec{r}$, $\psi(|\mathbf{r}|)$, has even parity.

2.4 TWO-PARTICLE SYSTEMS IN QUANTUM MECHANICS[6]

In considering the problem of a particle bound in a potential we assumed that the potential was a given function of position, which is equivalent to the statement that the particle moves under the action of an externally applied force. The symmetry properties possessed by the particle's "motion" (in quantum mechanical language, by its wave function), are then determined by the symmetry properties we have ascribed to the applied force. As in the classical case, however, the free play of natural laws can best be observed by considering instead two particles in mutual interaction.

We now show that the problem of two particles interacting with mutual forces, given by a potential which depends only on the position of one particle relative to the other, i.e.,

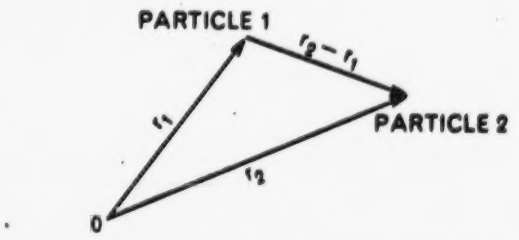

Fig. 2.4 Description of two-particle system.

$V(\vec{r}_2 - \vec{r}_1)$ where $\vec{r}_1$ and $\vec{r}_2$ are respectively the positions of particles 1 and 2 (see Fig. 2.4), reduces to the solution of a one-particle Schrödinger equation with a modified kinetic energy.

The two-particle system is described by a wave function $\psi(\vec{r}_1, \vec{r}_2)$ with the probability interpretation

$$P(\vec{r}_1, \vec{r}_2) = |\psi(\vec{r}_1, \vec{r}_2)|^2 \equiv \psi^*(\vec{r}_1, \vec{r}_2)\psi(\vec{r}_1, \vec{r}_2),$$

where $P(\vec{r}_1, \vec{r}_2)dV_1 dV_2$ is the probability of finding particle 1 within the volume dV_1 located at $\vec{r}_1$ and simultaneously finding particle 2 within the volume dV_2 located at $\vec{r}_2$. The wave function $\psi(\vec{r}_1, \vec{r}_2)$ satisfies the Schrödinger equation (for total energy E):

$$\left[-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V(\vec{r}_2 - \vec{r}_1)\right] \times \psi(\vec{r}_1, \vec{r}_2) = E\psi(\vec{r}_1, \vec{r}_2) \tag{2.27}$$

The symbol ∇_1^2 means $(d^2/dx_1^2) + (d^2/dy_1^2) + (d^2/dz_1^2)$ where $\vec{r}_1$ has components x_1, y_1, z_1 and similarly for ∇_2^2, which refers to the coordinates of particle 2.

We now introduce two new vector coordinates:

$\vec{R}$, the coordinate of the center of mass

and

$\vec{\rho} = \vec{r}_2 - \vec{r}_1$, the relative coordinate of 2 with respect to 1.

[6] This section is somewhat more difficult than the others, and it is not essential for the further development. However, the reader who knows partial derivatives should read it at this point.

By definition,

$$\vec{R} = \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2} . \qquad (2.28)$$

Letting the total mass $m_1 + m_2 = M$, and defining the reduced mass μ by

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} , \qquad (2.29)$$

we have

$$\mu = \frac{m_1 m_2}{M} . \qquad (2.30)$$

To complete the notation, we let $\vec{\rho}$ have coordinates ξ, η, ζ so that

$$\begin{aligned} \xi &= x_2 - x_1 \\ \eta &= y_2 - y_1 \\ \zeta &= z_2 - z_1 , \end{aligned} \qquad (2.31)$$

and we let $\vec{R}$ have coordinates X, Y, Z, so that

$$\begin{aligned} X &= \frac{m_1}{M} x_1 + \frac{m_2}{M} x_2 \\ Y &= \frac{m_1}{M} y_1 + \frac{m_2}{M} y_2 \\ Z &= \frac{m_1}{M} z_1 + \frac{m_2}{M} z_2 . \end{aligned} \qquad (2.32)$$

Notice that the x components, ξ and X, of $\vec{\rho}$ and $\vec{R}$ depend only on x_1 and x_2 and not, for example, on y_1 or z_2. We are thus able to express x_1 and x_2, and $\partial/\partial x_1$, $\partial^2/\partial x_1^2$, $\partial/\partial x_2$, $\partial^2/\partial x_2^2$ in terms of ξ and X. We get

$$\begin{aligned} \frac{\partial}{\partial x_1} &= \frac{\partial \xi}{\partial x_1} \frac{\partial}{\partial \xi} + \frac{\partial X}{\partial x_1} \frac{\partial}{\partial X} \\ &= - \frac{\partial}{\partial \xi} + \frac{m_1}{M} \frac{\partial}{\partial X} \end{aligned} \qquad (2.33)$$

and

$$\begin{aligned} \frac{\partial^2}{\partial x_1^2} &= \frac{\partial}{\partial x_1}\left(\frac{\partial}{\partial x_1}\right) = \left(- \frac{\partial}{\partial \xi} + \frac{m_1}{M} \frac{\partial}{\partial X}\right) \\ &\times \left(- \frac{\partial}{\partial \xi} + \frac{m_1}{M} \frac{\partial}{\partial X}\right) = \frac{\partial^2}{\partial \xi^2} + \frac{m_1^2}{M^2} \frac{\partial^2}{\partial X^2} \\ &- \frac{2m_1}{M} \frac{\partial}{\partial \xi} \frac{\partial}{\partial X} . \end{aligned} \qquad (2.34)$$

Similar expressions are obtained for $\partial^2/\partial x_2^2$, etc.

We now consider the first two terms in the bracket of Eq. (2.27)

$$\begin{aligned} &- \frac{\hbar^2}{2m_1} \nabla_1^2 - \frac{\hbar^2}{2m_2} \nabla_2^2 = \\ &- \frac{\hbar^2}{2} \left\{ \frac{1}{m_1} \frac{\partial^2}{\partial x_1^2} + \frac{1}{m_2} \frac{\partial^2}{\partial x_2^2} \right. \\ &+ \frac{1}{m_1} \frac{\partial^2}{\partial y_1^2} + \frac{1}{m_2} \frac{\partial^2}{\partial y_2^2} \\ &\left. + \frac{1}{m_1} \frac{\partial^2}{\partial z_1^2} + \frac{1}{m_2} \frac{\partial^2}{\partial z_2^2} \right\} . \end{aligned} \qquad (2.35)$$

Take the part

$$\frac{1}{m_1} \frac{\partial^2}{\partial x_1^2} + \frac{1}{m_2} \frac{\partial^2}{\partial x_2^2} , \qquad (2.36)$$

which is, according to Eq. (2.34)

$$\begin{aligned} &\frac{1}{m_1}\left[\frac{\partial^2}{\partial \xi^2} + \frac{m_1^2}{M^2} \frac{\partial^2}{\partial X^2} - 2\frac{m_1}{M} \frac{\partial}{\partial \xi} \frac{\partial}{\partial X}\right] \\ &+ \frac{1}{m_2}\left[\frac{\partial^2}{\partial \xi^2} + \frac{m_2^2}{M^2} \frac{\partial^2}{\partial X^2} + 2\frac{m_2}{M} \frac{\partial}{\partial \xi} \frac{\partial}{\partial X}\right] , \end{aligned} \qquad (2.37)$$

where the change of sign in the second bracket is traceable to the definition in Eq. (2.31) where x_1, y_1, z_1 have the negative sign. In combining the terms in the two brackets of Eq. (2.37) it will be seen that the terms containing mixed derivatives cancel, and we get

$$\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\frac{\partial^2}{\partial \xi^2} + \frac{m_1 + m_2}{M^2} \frac{\partial^2}{\partial X^2} , \qquad (2.38)$$

or

$$\frac{1}{\mu} \frac{\partial^2}{\partial \xi^2} + \frac{1}{M} \frac{\partial^2}{\partial X^2} , \qquad (2.39)$$

on recalling the definitions of μ and M. Similar expressions are obtained for the other parts of Eq. (2.35) so that we have finally:

$$-\frac{\hbar^2}{2m}\nabla_1^2-\frac{\hbar^2}{2m_2}\nabla_2^2$$

$$=-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}+\frac{\partial^2}{\partial\xi^2}\right)$$

$$-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial X^2}+\frac{\partial^2}{\partial Y^2}+\frac{\partial^2}{\partial Z^2}\right)$$

$$=-\frac{\hbar^2}{2\mu}\nabla_\rho^2-\frac{\hbar^2}{2M}\nabla_R^2.$$

The Schrödinger equation (2.27) is thus equivalent to the two Schrödinger equations:

$$-\frac{\hbar^2}{2M}\nabla_R^2F(\vec{R})=E_RF(\vec{R}), \qquad (2.40a)$$

$$-\frac{\hbar^2}{\partial\mu}\nabla_\rho^2G(\vec{\rho})+V(\vec{\rho})G(\vec{\rho})=E_\rho G(\vec{\rho}), \qquad (2.40b)$$

where $\psi(\vec{r}_1,\vec{r}_2)=F(\vec{R})G(\vec{\rho})$ and $E_R+E_\rho=E$.

Equation (2.40a), which describes the motion of the center of mass of the two-particle system, is the equation for a free "particle." Its solution is

$$F(\vec{R})=A\exp\left(\frac{i}{\hbar}\vec{P}\cdot\vec{R}\right), \qquad (2.41)$$

which reduces to the constant A in the center-of-mass system, that is, that system in which the total momentum $\vec{P}$ (and hence E_R) is zero. Since we are primarily interested in the mutual interaction of the two particles, we usually work in this reference system. In this case we deal with Eq. (2.40b) alone, which is a "one-particle" Schrödinger equation, with "mass" μ, the reduced mass, as the "particle" mass.

Appendix GROUP ALGEBRA

Consider the "minimum set of operations" discussed in the text by which the equilateral triangle can be brought into congruence with itself. This particular minimum set consists of:

Clockwise rotation about the center of the triangle by 120° (called R).

Clockwise rotation about the center of the triangle by 240° (called R^2 because it is equivalent to R performed twice in succession), leaving the triangle alone (called I, standing for "identity"), flipping about an axis, say the angle bisector of the lower left hand vertex angle (called F).

For the moment, let us only consider the rotations, and not the flipping. The operation R, repeated twice is written RR. As we have noted above, this is equivalent to the operation R^2. Similarly $R \cdot R^2$ means performing R^2 first, then R (we read operations from the right to the left), while $R^2 \cdot R$ means performing R first, then R^2. Evidently,

$$R \cdot R^2 = R^2 \cdot R = R^3 = I.$$

The rotations alone have the properties required to form what mathematicians call a group:

(a) There is a set of operations (R, R^2, I) called group elements and a rule for combining them (that is, successively performing them). We call the successive performance $R \cdot R^2$ (that is, first R^2, then R), multiplication of R^2 by R on the left or multiplication of R by R^2 on the right.

(b) If we consider $R \cdot R \cdot R$, the result may be written $R \cdot R^2$ or $R^2 \cdot R$, or to take another example we can write RRI as R^2I or $R(RI) = R \cdot R$. That is, multiplication is associative.

(c) There is an identity element I.

(d) R^2 and R are inverses in the sense that $R^2R = I$ and $RR^2 = I$.

(e) Any product of R, R^2, I is again one of these three, for example:

$$R = R^4 = R^7 = \ldots$$

$$R^2 = R^5 = R^8 = \ldots$$

$$I = R^3 = R^6 = R^9 = \ldots$$

The set of elements R, R^2, I is closed under multiplication.[7]

Although the elements I, R, and R^2 form a group, they form part of another larger group which can be obtained by considering them in combination with the element F. We say that I, R, and R^2 form a subgroup of the larger group, which consists of I, R, R^2, FI = F, FR, and FR^2. To show that this set of six elements form a group, and to exhibit the group properties, we make a group multiplication table. Note first that the element FR is not equal to RF, and that, in general, left multiplication is not equivalent to right multiplication. This can be seen by actually performing the operations in order, starting from the right. In this way the reader can verify, in fact, that $RF = FR^2$. In the multiplication table (facing page), the elements in the left-hand column are multiplied by those in the top row to obtain the entry at the intersection.

In making the table we have simplified the results so that only group elements appear in the table. For ex-

[7] A group consisting of only a single element (like R) and its powers is called a cyclic group. Evidently there consists a cyclic group of four elements (the 90° rotations) and, in fact, of five, six, . . . elements. To what do they correspond geometrically?

ample, in obtaining R·FR, we have used $RF = FR^2$, hence

$$R \cdot FR = RF \cdot R = FR^2 \cdot R = FR^3 = FI = F.$$

Similarly,

$$R \cdot FR^2 = RF \cdot R^2 = FR^2 \cdot R^2 = FR^4 = FR.$$

Since only group elements appear in the table, we have proven that the six elements chosen are <u>closed</u> under group multiplication. There is an identity element I, and each element can be seen from the table to have an inverse in the set. Therefore, they form a group.

The group of six elements having the multiplication table shown is sometimes called the permutation group on three letters, since the six positions of the equilateral triangle shown in Fig. 1.2 correspond to the six possible arrangements or permutations of the letters ABC which label the vertices.

MULTIPLICATION TABLE

	I	R	R^2	F	FR	FR^2
I	I	R	R^2	F	FR	FR^2
R	R	R^2	I	FR^2	F	FR
R^2	R^2	I	R	FR	FR^2	F
F	F	FR	FR^2	I	R	R^2
FR	FR	FR^2	F	R^2	I	R
FR^2	FR^2	F	FR	R	R^2	I